Christoph Dellago

List of Publications by Year
in descending order

194	12,666	41258	25716
papers	citations	49 h-index	108 g-index

199	199	199	8974
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	TRANSITIONPATHSAMPLING: Throwing Ropes Over Rough Mountain Passes, in the Dark. Annual Review of Physical Chemistry, 2002, 53, 291-318.	4.8	1,704
2	Transition path sampling and the calculation of rate constants. Journal of Chemical Physics, 1998, 108, 1964-1977.	1.2	925
3	Accurate determination of crystal structures based on averaged local bond order parameters. Journal of Chemical Physics, 2008, 129, 114707.	1.2	707
4	Autoionization in Liquid Water. Science, 2001, 291, 2121-2124.	6.0	672
5	Reaction coordinates of biomolecular isomerization. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 5877-5882.	3.3	370
6	Proton Transport through Water-Filled Carbon Nanotubes. Physical Review Letters, 2003, 90, 105902.	2.9	339
7	Efficient transition path sampling: Application to Lennard-Jones cluster rearrangements. Journal of Chemical Physics, 1998, 108, 9236-9245.	1.2	313
8	How van der Waals interactions determine the unique properties of water. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8368-8373.	3.3	312
9	Kinetic Pathways of Ion Pair Dissociation in Water. Journal of Physical Chemistry B, 1999, 103, 3706-3710.	1.2	310
10	Transition Path Sampling. Advances in Chemical Physics, 2003, , 1-78.	0.3	310
11	On the calculation of reaction rate constants in the transition path ensemble. Journal of Chemical Physics, 1999, 110, 6617-6625.	1.2	292
12	Sampling ensembles of deterministic transition pathways. Faraday Discussions, 1998, 110, 421-436.	1.6	282
13	Direct Measurement of Photon Recoil from a Levitated Nanoparticle. Physical Review Letters, 2016, 116, 243601.	2.9	239
14	Ab initio thermodynamics of liquid and solid water. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 1110-1115.	3.3	201
15	Melting of icosahedral gold nanoclusters from molecular dynamics simulations. Journal of Chemical Physics, 2005, 122, 214722.	1.2	194
16	Library-Based LAMMPS Implementation of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 1827-1840.	2.3	175
17	Biased Sampling of Nonequilibrium Trajectories:Â Can Fast Switching Simulations Outperform Conventional Free Energy Calculation Methods?â€. Journal of Physical Chemistry B, 2005, 109, 6902-6915.	1.2	151
18	Dynamic relaxation of a levitated nanoparticle from a non-equilibrium steady state. Nature Nanotechnology, 2014, 9, 358-364.	15.6	151

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19	Macroscopically ordered water in nanopores. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13218-13222.	3.3	145
20	Lyapunov instability in a system of hard disks in equilibrium and nonequilibrium steady states. Physical Review E, 1996, 53, 1485-1501.	0.8	143
21	Parallel Multistream Training of High-Dimensional Neural Network Potentials. Journal of Chemical Theory and Computation, 2019, 15, 3075-3092.	2.3	124
22	Role of the Prestructured Surface Cloud in Crystal Nucleation. Physical Review Letters, 2011, 106, 085701.	2.9	122
23	Neural networks for local structure detection in polymorphic systems. Journal of Chemical Physics, 2013, 139, 164105.	1.2	115
24	Molecular mechanism for cavitation in water under tension. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13582-13587.	3.3	110
25	An enhanced version of the heat exchange algorithm with excellent energy conservation properties. Journal of Chemical Physics, 2015, 143, 124104.	1.2	108
26	Direct measurement of Kramers turnover with a levitated nanoparticle. Nature Nanotechnology, 2017, 12, 1130-1133.	15.6	102
27	Single-file water in nanopores. Physical Chemistry Chemical Physics, 2011, 13, 15403.	1.3	99
28	Mechanisms of the Wurtzite to Rocksalt Transformation in CdSe Nanocrystals. Physical Review Letters, 2006, 96, 255701.	2.9	98
29	Carâ€“Parrinello molecular dynamics simulation of the calcium ion in liquid water. Chemical Physics Letters, 2003, 369, 159-164.	1.2	85
30	Kinetics and Mechanism of Proton Transport across Membrane Nanopores. Physical Review Letters, 2006, 97, 245901.	2.9	84
31	Largest Lyapunov Exponent for Many Particle Systems at Low Densities. Physical Review Letters, 1998, 80, 2035-2038.	2.9	81
32	Melting and equilibrium shape of icosahedral gold nanoparticles. Chemical Physics Letters, 2004, 394, 257-261.	1.2	73
33	Surface-Driven Bulk Reorganization of Gold Nanorods. Nano Letters, 2005, 5, 2174-2178.	4.5	69
34	Transition Path Sampling and Other Advanced Simulation Techniques for Rare Events. , 2009, , 167-233.		69
35	Equilibrium free energies from fast-switching trajectories with large time steps. Journal of Chemical Physics, 2006, 124, 044113.	1.2	66
36	Transition Path Sampling Simulations of Biological Systems. , 2006, , 291-317.		64

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37	Computing Gibbs free energy differences by interface pinning. Physical Review B, 2013, 88, .	1.1	64
38	Structural and Morphological Transitions in Gold Nanorods:Â A Computer Simulation Study. Journal of Physical Chemistry B, 2003, 107, 9214-9219.	1.2	62
39	Kolmogorov-Sinai entropy for dilute gases in equilibrium. Physical Review E, 1997, 56, 5272-5277.	0.8	61
40	Chemical dynamics of the protonated water trimer analyzed by transition path sampling. Physical Chemistry Chemical Physics, 1999, 1, 1317-1322.	1.3	61
41	Computing Equilibrium Free Energies Using Non-Equilibrium Molecular Dynamics. Entropy, 2014, 16, 41-61.	1.1	60
42	Kolmogorov-Sinai entropy and Lyapunov spectra of a hard-sphere gas. Physica A: Statistical Mechanics and Its Applications, 1997, 240, 68-83.	1.2	59
43	Perspectives on the Future of Ice Nucleation Research: Research Needs and Unanswered Questions Identified from Two International Workshops. Atmosphere, 2017, 8, 138.	1.0	56
44	Mechanism of alkane dehydrogenation catalyzed by acidic zeolites: Ab initio transition path sampling. Journal of Chemical Physics, 2009, 131, 214508.	1.2	55
45	Sequence Controlled Self-Knotting Colloidal Patchy Polymers. Physical Review Letters, 2013, 110, 075501.	2.9	55
46	Ab initio analysis of proton transfer dynamics in (H2O)3H+. Chemical Physics Letters, 2000, 321, 225-230.	1.2	54
47	Toward the Mechanism of Ionic Dissociation in Water. Journal of Physical Chemistry B, 2012, 116, 13490-13497.	1.2	54
48	Calibration and energy measurement of optically levitated nanoparticle sensors. Review of Scientific Instruments, 2018, 89, 033111.	0.6	54
49	Transition path sampling: throwing ropes over mountains in the dark. Journal of Physics Condensed Matter, 2000, 12, A147-A152.	0.7	52
50	Wang-Landau sampling with self-adaptive range. Physical Review E, 2005, 71, 066705.	0.8	52
51	Diffusion of isobutane in silicalite studied by transition path sampling. Journal of Chemical Physics, 2000, 113, 8791-8799.	1.2	51
52	Crystallization of a binary Lennard-Jones mixture. Journal of Chemical Physics, 2011, 134, 104501.	1.2	50
53	Nucleation and Growth in Structural Transformations of Nanocrystals. Nano Letters, 2009, 9, 2099-2102.	4.5	49
54	Practical and conceptual path sampling issues. European Physical Journal: Special Topics, 2015, 224, 2409-2427.	1.2	48

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55	Melting Si: Beyond Density Functional Theory. Physical Review Letters, 2018, 121, 195701.	2.9	46
56	Lyapunov instability, local curvature, and the fluid-solid phase transition in two-dimensional particle systems. Physica A: Statistical Mechanics and Its Applications, 1996, 230, 364-387.	1.2	41
57	Reaction coordinates for the crystal nucleation of colloidal suspensions extracted from the reweighted path ensemble. Journal of Chemical Physics, 2011, 135, 154110.	1.2	40
58	Long-Range Dispersion Effects on the Water/Vapor Interface Simulated Using the Most Common Models. Journal of Physical Chemistry B, 2017, 121, 3798-3803.	1.2	40
59	Lyapunov exponents of systems with elastic hard collisions. Physical Review E, 1995, 52, 2401-2406.	0.8	39
60	The statistics of electric field fluctuations in liquid water. Molecular Physics, 2009, 107, 495-502.	0.8	39
61	Free energies of theÏ•4model from Wang-Landau simulations. Physical Review B, 2005, 72, .	1.1	37
62	A proof of Jarzynskiâ€™s nonequilibrium work theorem for dynamical systems that conserve the canonical distribution. Journal of Chemical Physics, 2006, 125, 054105.	1.2	37
63	Precision shooting: Sampling long transition pathways. Journal of Chemical Physics, 2008, 129, 194101.	1.2	37
64	Dynamical Aspects of Isomerization and Melting Transitions in [H2O]8â€. Journal of Physical Chemistry A, 2001, 105, 2646-2651.	1.1	36
65	Optimum protocol for fast-switching free-energy calculations. Physical Review E, 2010, 81, 021127.	0.8	36
66	Pathways to self-organization: Crystallization via nucleation and growth. European Physical Journal E, 2016, 39, 77.	0.7	36
67	Lyapunov Exponents from Kinetic Theory for a Dilute, Field-Driven Lorentz Gas. Physical Review Letters, 1996, 77, 1974-1977.	2.9	35
68	Density-Dependent Diffusion in the Periodic Lorentz Gas. Journal of Statistical Physics, 2000, 101, 145-159.	0.5	35
69	Proton Ordering of Cubic Ice Ic: Spectroscopy and Computer Simulations. Journal of Physical Chemistry C, 2014, 118, 10989-10997.	1.5	35
70	Activation Energies from Transition Path Sampling Simulations. Molecular Simulation, 2004, 30, 795-799.	0.9	33
71	Optimising reaction coordinates for crystallisation by tuning the crystallinity definition. Molecular Physics, 2013, 111, 3527-3533.	0.8	33
72	On the efficiency of path sampling methods for the calculation of free energies from non-equilibrium simulations. Journal of Statistical Mechanics: Theory and Experiment, 2007, 2007, P04001-P04001.	0.9	32

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73	On the accuracy of the size distribution information obtained from light extinction and scattering measurementsâ€"I. Basic considerations and models. Journal of Aerosol Science, 1993, 24, 129-141.	1.8	31
74	Lyapunov spectrum of the driven Lorentz gas. Physical Review E, 1995, 52, 4817-4826.	0.8	31
75	Dynamic phases of colloidal monolayers sliding on commensurate substrates. Soft Matter, 2013, 9, 5867.	1.2	31
76	Simulation strategies and signatures of chaos in classical nonlinear response. Physical Review E, 2003, 67, 035205.	0.8	29
77	Non-equilibrium steady state of a driven levitated particle with feedback cooling. New Journal of Physics, 2015, 17, 045011.	1.2	29
78	Mixing, Lyapunov instability, and the approach to equilibrium in a hard-sphere gas. Physical Review E, 1997, 55, R9-R12.	0.8	28
79	Lyapunov Modes of Two-Dimensional Many-Body Systems; Soft Disks, Hard Disks, and Rotors. Journal of Statistical Physics, 2002, 109, 765-776.	0.5	28
80	Design and folding of colloidal patchy polymers. Soft Matter, 2013, 9, 938-944.	1.2	28
81	Simulation algorithms for multidimensional nonlinear response of classical many-body systems. Journal of Chemical Physics, 2003, 119, 9344-9354.	1.2	27
82	Orientational Dynamics and Dielectric Response of Nanopore Water. Physical Review Letters, 2009, 103, 080601.	2.9	27
83	Lyapunov Spectrum and the Conjugate Pairing Rule for a Thermostatted Random Lorentz Gas: Numerical Simulations. Physical Review Letters, 1997, 78, 211-214.	2.9	26
84	Equilibrium Time Correlation Functions from Irreversible Transformations in Trajectory Space. Journal of Physical Chemistry B, 2004, 108, 6667-6672.	1.2	26
85	An efficient transition path sampling algorithm for nanoparticles under pressure. Journal of Chemical Physics, 2007, 127, 154718.	1.2	26
86	Defect interactions in two-dimensional colloidal crystals: vacancy and interstitial strings. Soft Matter, 2009, 5, 2752.	1.2	25
87	Nanoparticle-based crystal growth via multistep self-assembly. CrystEngComm, 2013, 15, 5114.	1.3	25
88	Theoretical prediction of the homogeneous ice nucleation rate: disentangling thermodynamics and kinetics. Physical Chemistry Chemical Physics, 2018, 20, 28732-28740.	1.3	25
89	A one-dimensional dipole lattice model for water in narrow nanopores. Journal of Chemical Physics, 2009, 130, 154110.	1.2	24
90	Simulating rare switching events of magnetic nanostructures with forward flux sampling. Physical Review B, 2013, 88, .	1.1	24

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91	Ab initio structure and thermodynamics of the RPBE-D3 water/vapor interface by neural-network molecular dynamics. Journal of Chemical Physics, 2020, 153, 144710.	1.2	24
92	On the accuracy of the size distribution information obtained from light extinction and scattering measurementsâ€"II. Case studies. Journal of Aerosol Science, 1993, 24, 143-154.	1.8	23
93	Potential energy landscape for proton transfer in (H2O)3H+: comparison of density functional theory and wavefunction-based methods. Chemical Physics Letters, 2000, 324, 149-155.	1.2	23
94	Transition Path Sampling Methods. , 2006, , 349-391.		23
95	Single molecule pulling with large time steps. Physical Review E, 2007, 75, 061106.	0.8	23
96	Biasing the Center of Charge in Molecular Dynamics Simulations with Empirical Valence Bond Models:â€‰ Free Energetics of an Excess Proton in a Water Droplet. Journal of Physical Chemistry B, 2008, 112, 2349-2356.	1.2	23
97	Lyapunov instability in the extended XY-model: Equilibrium and nonequilibrium molecular dynamics simulations. Physica A: Statistical Mechanics and its Applications, 1997, 237, 95-112.	1.2	22
98	Ideal gas pressure bath: a method for applying hydrostatic pressure in the computer simulation of nanoparticles. Molecular Physics, 2006, 104, 3709-3715.	0.8	22
99	Gas-phase formation of large neutral alkaline-earth metal tryptophan complexes. Journal of the American Society for Mass Spectrometry, 2008, 19, 1021-1026.	1.2	22
100	Dipole moment of water molecules in narrow pores. Computer Physics Communications, 2005, 169, 36-39.	3.0	21
101	Point defects in two-dimensional colloidal crystals: simulation vs. elasticity theory. Soft Matter, 2009, 5, 646-659.	1.2	21
102	Heterogeneous crystallization on tiny clusters. Europhysics Letters, 2011, 96, 56006.	0.7	21
103	Crystallization on prestructured seeds. Physical Review E, 2013, 87, 012305.	0.8	21
104	Self-assembly of DNA-functionalized colloids. Condensed Matter Physics, 2015, , 22801.	0.3	21
105	Transition state analysis of solid-solid transformations in nanocrystals. Journal of Chemical Physics, 2009, 131, 164116.	1.2	20
106	Single-file water as a one-dimensional Ising model. New Journal of Physics, 2010, 12, 093044.	1.2	20
107	A coarse-grained model for DNA-functionalized spherical colloids, revisited: Effective pair potential from parallel replica simulations. Journal of Chemical Physics, 2013, 138, 025101.	1.2	20
108	Identifying rare chaotic and regular trajectories in dynamical systems with Lyapunov weighted path sampling. Chemical Physics, 2010, 375, 309-315.	0.9	19

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109	Detecting vapour bubbles in simulations of metastable water. Journal of Chemical Physics, 2014, 141, 18C511.	1.2	19
110	Folding mechanism of a polymer chain with short-range attractions. Journal of Chemical Physics, 2014, 141, 134901.	1.2	19
111	Optimum bias for fast-switching free energy calculations. Computer Physics Communications, 2008, 179, 41-45.	3.0	18
112	The role of directional interactions in the designability of generalized heteropolymers. Scientific Reports, 2017, 7, 4986.	1.6	18
113	Role of Water in the Selection of Stable Proteins at Ambient and Extreme Thermodynamic Conditions. Physical Review X, 2017, 7, .	2.8	18
114	Hierarchical self-assembly of patchy colloidal platelets. Soft Matter, 2020, 16, 2774-2785.	1.2	18
115	Transition Path Sampling. , 2005, , 1585-1596.		18
116	Finite-precision stationary states at and away from equilibrium. Physical Review E, 2000, 62, 6275-6281.	0.8	17
117	Non-equilibrium simulations of thermally induced electric fields in water. Journal of Chemical Physics, 2016, 144, 224102.	1.2	17
118	Design of Patchy Rhombi: From Close-Packed Tilings to Open Lattices. Nano Letters, 2019, 19, 7806-7815.	4.5	17
119	Dissociation of Hydrogen Chloride and Proton Transfer in Liquid Glycerol:Â An Ab Initio Molecular Dynamics Studyâ€. Journal of Physical Chemistry B, 2004, 108, 19647-19656.	1.2	16
120	Efficient extraction of free energy profiles from nonequilibrium experiments. Journal of Computational Chemistry, 2009, 30, 1726-1736.	1.5	16
121	Overcoming barriers in trajectory space: Mechanism and kinetics of rare events via Wangâ€“Landau enhanced transition path sampling. Journal of Chemical Physics, 2010, 133, 134112.	1.2	16
122	Time-reversal symmetry and covariant Lyapunov vectors for simple particle models in and out of thermal equilibrium. Physical Review E, 2010, 82, 046218.	0.8	16
123	Phase Transition and Interpore Correlations of Water in Nanopore Membranes. Physical Review Letters, 2012, 109, 020602.	2.9	15
124	Self-organized defect strings in two-dimensional crystals. Physical Review E, 2013, 88, 060402.	0.8	15
125	Computing the crystal growth rate by the interface pinning method. Journal of Chemical Physics, 2015, 142, 044104.	1.2	15
126	Optimizing transition interface sampling simulations. Journal of Chemical Physics, 2011, 134, 244118.	1.2	14

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127	Effect of entropy on the nucleation of cavitation bubbles in water under tension. Journal of Chemical Physics, 2016, 145, 211918.	1.2	14
128	A High Coordination of Cross-Links Is Beneficial for the Strength of Cross-Linked Fibers. Biomimetics, 2019, 4, 12.	1.5	13
129	Consequences of Lattice Mismatch for Phase Equilibrium in Heterostructured Solids. Physical Review Letters, 2019, 123, 135701.	2.9	13
130	Coarse Graining the Ït‹sup›4‹/sup›Model: Landau-Ginzburg Potentials from Computer Simulations. Ferroelectrics, 2007, 354, 225-237.	0.3	12
131	Frictional dynamics of stiff monolayers: from nucleation dynamics to thermal sliding. Nanoscale, 2014, 6, 10161-10168.	2.8	12
132	Calculating thermal stability and attempt frequency of advanced recording structures without free parameters. Journal of Applied Physics, 2015, 117, 163907.	1.1	12
133	Interplay of fast and slow dynamics in rare transition pathways: The disk-to-slab transition in the 2d Ising model. Journal of Chemical Physics, 2017, 147, 152714.	1.2	12
134	Numerical evidence for thermally induced monopoles. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 4911-4914.	3.3	11
135	Effect of Surface Structure on Shape Transformations of Gold Nanorods. Journal of Computational and Theoretical Nanoscience, 2007, 4, 282-290.	0.4	10
136	S-shooting: a Bennettâ€“Chandler-like method for the computation of rate constants from committor trajectories. Faraday Discussions, 2016, 195, 345-364.	1.6	10
137	Density anomaly of water at negative pressures from first principles. Journal of Physics Condensed Matter, 2018, 30, 254005.	0.7	10
138	Improved description of atomic environments using low-cost polynomial functions with compact support. Machine Learning: Science and Technology, 2021, 2, 035026.	2.4	10
139	Are local Lyapunov exponents continuous in phase space?. Physics Letters, Section A: General, Atomic and Solid State Physics, 2000, 268, 330-334.	0.9	9
140	Comment on â€œDissociation of Water under Pressureâ€• Physical Review Letters, 2002, 89, 199601; author reply 199602.	2.9	9
141	Microscopic properties of nanopore water from its time-dependent dielectric response. Physical Review B, 2010, 82, .	1.1	9
142	Vibrational Spectroscopy of Water in Narrow Nanopores. Journal of Physical Chemistry B, 2011, 115, 5268-5277.	1.2	9
143	Heteropolymer Design and Folding of Arbitrary Topologies Reveals an Unexpected Role of Alphabet Size on the Knot Population. Macromolecules, 2018, 51, 8346-8356.	2.2	9
144	Fluctuations, convergence times, correlation functions, and power laws from many-body Lyapunov spectra for soft and hard disks and spheres. Physical Review E, 2002, 65, 056216.	0.8	8

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145	Displacement fields of point defects in two-dimensional colloidal crystals. Journal of Physics Condensed Matter, 2008, 20, 404202.	0.7	8
146	The configurational space of colloidal patchy polymers with heterogeneous sequences. Journal of Physics Condensed Matter, 2012, 24, 284111.	0.7	8
147	General Methodology to Identify the Minimum Alphabet Size for Heteropolymer Design. Advanced Theory and Simulations, 2019, 2, 1900031.	1.3	8
148	Origin of mean-field behavior in an elastic Ising model. Physical Review B, 2020, 102, .	1.1	8
149	Demixing of a binary symmetric mixture studied with transition path sampling. Journal of Chemical Physics, 2010, 133, 104505.	1.2	7
150	Wired-up water. Nature Chemistry, 2012, 4, 245-247.	6.6	7
151	Caveats of mean first-passage time methods applied to the crystallization transition: Effects of non-Markovianity. Journal of Chemical Physics, 2015, 142, 064103.	1.2	7
152	Avoiding traps in trajectory space: Metadynamics enhanced transition path sampling. European Physical Journal: Special Topics, 2016, 225, 1609-1620.	1.2	7
153	Crystallization and flow in active patch systems. Soft Matter, 2017, 13, 930-936.	1.2	7
154	A Shapeâ€Induced Orientation Phase within 3D Nanocrystal Solids. Advanced Materials, 2018, 30, e1802078.	11.1	7
155	Isomorphic multifractal shear flows for hard disks via adiabatic and isokinetic nonequilibrium molecular dynamics. Physical Review E, 1998, 57, 4969-4975.	0.8	6
156	On the reaction coordinate for seeded crystallisation. Molecular Physics, 2015, 113, 2735-2741.	0.8	6
157	Nucleation and structural growth of cluster crystals. Journal of Chemical Physics, 2016, 145, 074504.	1.2	6
158	Theoretical Prediction of Thermal Polarization. Physical Review Letters, 2018, 120, 226001.	2.9	6
159	Rigid-lattice Monte Carlo study of nucleation kinetics in dilute bcc Fe-Cu alloys using statistical sampling techniques. Acta Materialia, 2018, 159, 429-438.	3.8	6
160	Bridging the Time Scale Gap with Transition Path Sampling. Lecture Notes in Physics, 2002, , 321-333.	0.3	6
161	The Fourier Monte Carlo Approach to Lattice Spin Models. Physics Procedia, 2010, 6, 106-116.	1.2	5
162	A string reaction coordinate for the folding of a polymer chain. Journal of Physics Condensed Matter, 2015, 27, 194126.	0.7	5

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163	State-dependent diffusion coefficients and free energies for nucleation processes from Bayesian trajectory analysis. Molecular Physics, 2018, 116, 2987-2997.	0.8	5
164	The microscopic mechanism of bulk melting of ice. Journal of Chemical Physics, 2021, 155, 124501.	1.2	5
165	Transition Path Sampling and the Calculation of Free Energies. Springer Series in Chemical Physics, 2007, , 249-276.	0.2	5
166	On the accuracy of the size distribution information obtained from spectral extinction/scattering measurements. Journal of Aerosol Science, 1990, 21, S155-S158.	1.8	4
167	Large timeâ€step, fastâ€switching free energy calculations with nonâ€symplectic integrators. Israel Journal of Chemistry, 2007, 47, 215-223.	1.0	4
168	Design of Proteinâ€“Protein Binding Sites Suggests a Rationale for Naturally Occurring Contact Areas. Journal of Chemical Theory and Computation, 2019, 15, 1383-1392.	2.3	4
169	Protein design under competing conditions for the availability of amino acids. Scientific Reports, 2020, 10, 2684.	1.6	4
170	Field and density dependence of the Lyapunov spectrum for the driven random Lorentz gas. Physica D: Nonlinear Phenomena, 1998, 112, 241-249.	1.3	3
171	Entropy and kinetics of point defects in two-dimensional dipolar crystals. Physical Review E, 2015, 91, 032304.	0.8	3
172	Heterogeneous Crystallization on Pairs of Pre-Structured Seeds. Journal of Physical Chemistry B, 2016, 120, 9230-9239.	1.2	3
173	Phase stability of the ice XVII-based CO2 chiral hydrate from molecular dynamics simulations. Journal of Chemical Physics, 2019, 151, 104502.	1.2	3
174	Weak scaling of the contact distance between two fluctuating interfaces with system size. Physical Review E, 2020, 102, 062801.	0.8	3
175	How patchiness controls the properties of chain-like assemblies of colloidal platelets. Journal of Physics Condensed Matter, 2020, 32, 204001.	0.7	3
176	Cation interstitial diffusion in lead telluride and cadmium telluride studied by means of neural network potential based molecular dynamics simulations. Journal of Physics Condensed Matter, 2021, 33, 015901.	0.7	3
177	Nonlinear Response of Classical Dynamical Systems to Short Pulses. Bulletin of the Korean Chemical Society, 2003, 24, 1107-1110.	1.0	3
178	Catalytic Mechanism of Processive GlfT2: Transition Path Sampling Investigation of Substrate Translocation. ACS Omega, 2020, 5, 21374-21384.	1.6	3
179	Elastic forces drive nonequilibrium pattern formation in a model of nanocrystal ion exchange. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	3
180	Field-dependent collision frequency of the two-dimensional driven random Lorentz gas. Physical Review E, 2001, 64, 036217.	0.8	2

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181	Monte Carlo Sampling in Path Space: Calculating Time Correlation Functions by Transforming Ensembles of Trajectories. AIP Conference Proceedings, 2003, , .	0.3	2
182	New methods: general discussion. Faraday Discussions, 2016, 195, 521-556.	1.6	2
183	An efficient method to reconstruct free energy profiles for diffusive processes in transition interface sampling and forward flux sampling simulations. Journal of Chemical Physics, 2019, 150, 094114.	1.2	2
184	Enhancing transport by shaping barriers. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 2238-2240.	3.3	2
185	Transition Path Sampling Studies of Solid-Solid Transformations in Nanocrystals under Pressure. Challenges and Advances in Computational Chemistry and Physics, 2010, , 61-84.	0.6	2
186	A surface with variable reflectivity. Review of Scientific Instruments, 1990, 61, 1993-1994.	0.6	1
187	The Eighth Liquid Matter Conference. Journal of Physics Condensed Matter, 2012, 24, 280401.	0.7	1
188	Dynamical phases of attractive particles sliding on a structured surface. Journal of Physics Condensed Matter, 2015, 27, 194122.	0.7	1
189	Identification of Protein Functional Regions. ChemPhysChem, 2020, 21, 335-347.	1.0	1
190	The generic unfolding of a biomimetic polymer during force spectroscopy. Soft Matter, 2020, 16, 3941-3951.	1.2	1
191	The Eighth Liquid Matter Conference. Journal of Physics Condensed Matter, 2012, 24, 280301.	0.7	0
192	A Statistical Methodology to Reconstruct Nucleation Pathways in the Fe-Cu System. Materials Science Forum, 2016, 879, 1529-1534.	0.3	0
193	Nanocrystals: A Shape-Induced Orientation Phase within 3D Nanocrystal Solids (Adv. Mater. 32/2018). Advanced Materials, 2018, 30, 1870235.	11.1	0
194	Transition Path Sampling. , 2005, , 1585-1596.		0